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Some methodological aspects of mathematical modeling in dynamic systems

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Abstract: This paper is devoted to methodologies in the field of mathematical foundations of information technology and computer sciences. The theoretical foundations of mathematical modeling of dynamic systems are briefly presented. Various aspects of the concept of a model are considered. The division into types of models is presented. The steps of the mathematical modeling process are detailed. Basic requirements for mathematical models are formulated. The main approaches used in the process of mathematical modeling are described.
Keywords: Complex dynamical systems, Modeling, Methodology, Design.

1. Introduction

One of the new scientific directions that has appeared recently is mathematical modeling [1-5]. If in such classical scientific areas as mathematical analysis, geometry, differential equations, the basic mathematical apparatus used to obtain new results has already been formed, then the theory of mathematical modeling, as a separate scientific direction, it is just beginning to take shape. Although many interesting results are already known in various disciplinary fields: engineering [6-8], chemistry, chemical technology and production [2,9,], biology [10-12], economics and ecology [13,14]. In all these works, it is shown how to use the knowledge of each specific field as much as possible to apply it to the construction of a mathematical model of a particular process. In principle, for an experienced scientist, building a simple mathematical model is not too difficult task, and the result can be ambiguous. It is much more difficult to choose one single mathematical model which, on the one hand-side, is quite simple to study, and on the other, most adequately describes the real process. But, as experience shows, for a beginner, a senior student, a graduate, the task of constructing a model turns out to be extremely difficult (this means the stage of transition from a humane description to a formal mathematical abstraction record). Modern textbooks [15-18], which are primarily focused on the specifics of each subject area, and scientific works in which the principles are clearly formulated and the mathematical modeling process is written step by step, can help solve this problem.
Recently, a group of modeling methods has been widely developed, which are based on a multi-theoretical approach to the description of the behavior of dynamic systems, and allow the most effective use of computer technology as a tool of engineering calculation practice[19-24].

The paper outlines the main concepts and methods of mathematical modeling. An attempt was made to determine the structure of the theory and the main directions of its development.

2. Concept of model. Mathematical model

Modeling is the replacement of some objects (originals) with other objects (models) and the investigation of the properties of objects according to established models. Modeling theory is an interrelated set of provisions, definitions, methods and means of building and studying models. These provisions, definitions, methods and tools, as well as the models themselves, are the subject of modeling theory [1-5].

The term "model" is used widely and has various applications. An object model is usually understood as another object that imitates a certain set of properties of the object being modeled [1,16]. The model cannot and should not repeat all the characteristics of the original, otherwise the meaning of modeling is lost. The main goal when building a model is the possibility, by examining the model, to obtain results that can be applied to the original object.

The main purpose of modeling is to obtain an opportunity to study and analyze the functioning of individual characteristics of a real object. A real-world object has a huge number of properties and characteristics. But from the point of view of the purpose of the research, a small part of them is decisive. Therefore, the task of the researcher is to identify the main properties and transfer them to the model [1,15,16].

Types of models. Mathematical model. All models can be divided into two categories: experimental models and theoretical models. Theoretical models are formulated in the language of one or another subject area. There are physical, biological, economic models, etc [6-14]. From this series, we will select mathematical models. Today, in the practice of researchers, it is customary to write down a corresponding mathematical model based on the model of the subject field. The main advantage of a mathematical model is the ability to investigate the properties and behavior of the model in all or many situations, relying on the developed formal research methods. Using the developed mathematical apparatus, you can try to go beyond everyday logic and get qualitatively new results. And the accuracy of mathematical methods helps to determine the degree of adequacy of the obtained results.

In addition, computational experiments conducted using mathematical models allow for a more detailed and in-depth study of objects.

Mathematical modeling becomes especially significant when the object of research is in a single instance, the natural experiment takes a long time, or the price of the direct experiment is too high.

Creating a mathematical model can be considered a more creative than a formal act of the researcher, because several non-equivalent models can be written for the same object. The same object can be described using different mathematical apparatus. For example, choose a continuous or discrete, deterministic or stochastic model. This choice further determines both the research method and the possibility of obtaining certain results.

There are different approaches to creating a mathematical model, the results of which are two types of mathematical models: ***structural and functional*** models. The structural model simulates the internal structure of the object with some accuracy. When building such a model, the structure of the object is simplified in order to get an opportunity to study the model. As a result, it repeats the behavior of the object on some set of input influences.

To build a functional model, the results of observations of the modeled object in different situations under different influences are used. Analysis of the structure of the object is not carried out. Such a mathematical model will repeat the behavior of the object in those cases for which there are results of observations. One of the cases of this approach is the ***"black box"*** type model.

Both types of models have advantages and disadvantages. A functional model is usually easier to construct, but the model may lose its adequacy outside the domain of experimental research. On the other hand, a more complex structural approach allows you to try to create a model that will remain adequate in many situations.

3. The process of mathematical modeling

The process of mathematical modeling is quite complex. Each stage of it interacts with other stages, and the results of one stage determine the results and the possibility of carrying out others.

The process of mathematical modeling should be considered sequentially. But at each of the stages, the researcher can iteratively return to the previous stages until he is satisfied with the result in order to move on to the next one. At each iteration, errors are found and corrected, the degree of adequacy improves. At the stage of domain analysis, several models of different types can be recorded. But at the testing stage, the model type is rarely changed. If the process is satisfactory, then inadequacy should be detected in the early stages. At the last stages, you only need to increase the accuracy of some parameters.

Analysis of the subject area. One of the main stages determining the latter is the analysis of the situation. The process of mathematical modeling begins with the analysis of the subject area. At this stage, the object of research is determined, all components of the environment in which the object is located are distinguished, the influence of the environment and possible states of the object are analyzed.

Construction of the model. At the next stage, the model of the subject area is formulated. The research object is replaced by its model. This model describes which properties of the object are important from the researcher's point of view. If it is expected that a structural mathematical model will be built, then the structural components of the object, their relationships, types of input influences and output signals are described in the domain model.

Formulation of mathematical modeling problems. Next, they build a mathematical model. A mathematical model exists in the form of records using accepted mathematical symbols and reflects the properties of the object - the laws to which it is subject, the connections inherent in its component parts, etc.

Mathematical model research. Depending on the purpose of modeling and the subject description of the object, the mathematical model can be dynamic, that is, describe the dynamics of the process, and static, that is, in the form of ratios that do not change over time. Differential equations, algebraic or stochastic relations, etc. are used to write the model. For each type of model, the appropriate mathematical apparatus for the analysis of the obtained model is used. Using selected theoretical methods, new knowledge about the object can be obtained.

Computer simulation. As a rule, after developing a mathematical model, a numerical experiment is conducted. At the same time, a mathematical model is first prepared for a numerical experiment (differential equations are converted to discrete equations using difference schemes, the necessary statistics are collected, initial conditions are prepared, etc.). Next, numerical calculations of the model are carried out under various conditions and admissible initial values. The obtained results are being processed.

There is no need to argue about the significance of this stage in the modeling process. Today it occupies one of the leading places in terms of computer science and the IT industry. Its detailed consideration is beyond the scope of this article. If necessary, readers are invited to review the following literature and references therein [19-24].

Model testing. The degree of adequacy is determined, that is, the correspondence of the model to the modeled object. Adequacy means, on the one hand, a correct qualitative description of a real object. On the other hand, the model should correctly describe the object from a quantitative point of view according to the given characteristics with sufficient accuracy.

It is not reasonable to demand quantitative adequacy for all models. For example, for sociological or some economic models, an adequate description of the principles of behavior of social groups or economic agents, respectively, and not their quantitative characteristics, is important [13,14].

In addition, it is important to show that the already known laws of the subject area, which are known in advance, are fulfilled for the model. These can be phenomenological or semi-empirical laws of the subject area, such as Newton's law in physics, or results obtained using other research methods.

Analysis and interpretation of results. Based on the results of theoretical research and numerical experiments, it is necessary to formulate the results of the obtained research. These can be proven regularities, forecasts for the future, conditions for the effectiveness of certain management decisions, determination of the best (optimal) parameters of the functioning of the object (system), etc. Especially valuable is the search for some unexpected result, which was lucky to be obtained precisely due to the application of mathematical modeling and the use of mathematical research methods.

4. Basic requirements for the mathematical model

In the "Literature analysis" section, similar objects, methods of their research and improvement can be considered. You can give examples of objects and methods of research of other authors with the indication of the data of the authors and a link to this manuscript.

A mathematical model must satisfy certain requirements. They are mainly subjective in nature and are determined by the purpose of modeling and existing limitations. Let's consider some of them.

Adequacy. The model must satisfy the condition of adequacy with respect to the selected characteristics. Adequacy of the model means:

1. appropriate qualitative description of the object according to the selected characteristics. (for example, the stability of the movement of the model indicates the stability of the real object);
2. correct qualitative description with the appropriate degree of accuracy.

Thus, the adequacy of the model is determined not only by the object and the model, but also by a given set of simulated characteristics. Sometimes they talk about the degree of adequacy of the model, understanding by this the degree of truth of the model relative to the selected set of characteristics.

Factors not taken into account. When formulating a mathematical model, the researcher always neglects a number of factors that he considers insignificant. Other characteristics of the research object are idealized. There is a concept of model stability, which means the ability of the model to preserve its qualitative properties when its parameters or structure are disturbed. There is some scope for changing parameters.

Simplicity and optimality of the model. Simplicity means the amount of effort that the researcher must invest in studying the model. In general, simplicity and adequacy are contradictory properties. To improve adequacy, a cumbersome system with a large number of equations that are difficult to investigate may be required. The model is simple enough if modern research methods make it possible to conduct a qualitative and quantitative analysis of the selected characteristics at a reasonable cost and with sufficient accuracy to understand the result.

Hierarchy of variables. The significance of different variables and parameters may be different. Some of the variables that appear in the main dependencies are called primary, and others are called secondary.

The classification of variables according to the rate of change over time is especially important. When setting the problem, some characteristic values are determined - the main scales of the time scale and the space scale. Based on the given time scale, "normal", "slow" and "fast" variables are distinguished. In the future, slow variables can be taken into account in the model as parameters.

Quick variables are divided into short-term and long-term. The first can easily be replaced by average values. The others play an important role in the analysis of transient processes that connect one stationary mode to another.

By analogy, they propose a classification of variables according to the degree of spatial influence: "near", "far", "very far". In this way, some hierarchy of variables is established. Often, an effective method of solving such a problem can be the transition from a complex model with a large number of "microvariables" to a simpler model with a small number of "macrovariables". An example of such an approach is the transition from equations describing the trajectory of molecular motion to partial differential equations using the concepts of temperature and density [16].

Other requirements. Researchers note other factors affecting the properties and development of the model. These are, for example, phenomenological and semi-empirical laws. These laws exist in the subject area and the adequacy of the model depends on whether they are fulfilled.

One of the main questions that arises in the process of building a model is the question of the parameters characterizing the state of the object or process and the number of degrees of freedom, which is understood as the number of homogeneous scalar parameters. The number of parameters can be finite or infinite. Despite the fact that real objects usually have an infinite number of parameters, researchers try to work with a finite number because it makes analysis much easier.

5. Types of mathematical models and design methodology

The basis of modeling is the theory of similarity, which states that absolute similarity takes place only if one object is replaced by another, exactly the same. In modeling, absolute similarity has no place, it is only required that the model sufficiently adequately reflects the functioning properties of the object under investigation. Depending on the nature of the processes, types of mathematical modeling can be divided into deterministic and stochastic, static and dynamic, discrete, discrete-continuous and continuous. Deterministic modeling reflects deterministic processes, that is, processes in which the complete absence of random influences is assumed. Stochastic modeling reflects probabilistic events and processes. During modeling, a number of implementations of a random process are analyzed and its characteristics are evaluated, that is, a set of homogeneous implementations. Static modeling assumes the invariance of the studied phenomenon over time. A mathematical model is built that reflects the behavior of the object "as a whole". Dynamic modeling serves to describe the behavior of an object at any arbitrary variable moment in time. Discrete, discrete-continuous and continuous mathematical models are a specification of dynamic models. Systems of ordinary differential equations, systems of partial differential equations, difference equations, equations with aftereffect and integral equations are most often used. The mathematical model depends not only on the nature of the real object, but also on the tasks and capabilities of the researcher and the necessary reliability and accuracy of the solution to the problem.

At the present stage, the following approaches are used in the development of mathematical models.

Balanced approach. The basis of the balance approach is the assumption that the increase in the variable that describes the process is equal to the difference between the function that provides an increase in the number (the growth function) and the function that provides a decrease in the number (the mortality function). If we consider the period of time Δt , then

$$x(t+\Delta t)-x(t)=B(t,x(t),\Delta t)-D(t,x(t),\Delta t) \tag{1}$$

In this equation, $B(t,x(t),\Delta t)$ - the phase variable increases, and $D(t,x(t),\Delta t)$ - its decrease.

Hamiltonian (variational) approach. The best results in mathematical modeling of dynamic processes were obviously obtained in classical mechanics [2,9,16]. This is due, first of all, to historical features. All the first scientific works were related to sea navigation, planetary motion, etc. They developed a long time ago, so the mathematical apparatus for solving these problems is fully established. For the derivation of the equations of motion, Hamilton's formalism was proposed, which has proven itself well. It consists in the following. If the system in the phase space changes its state from the position x_0 at the instant of time t_0 to the position x_1 at the instant t_1, then the integral (sum) of the movements must be minimal

$$I[x(t)]=\int_{t_0}^{t_1} L(t,x(t),x'(t))dt \to \min \tag{2}$$

The function $L(t, x(t), x'(t))$ is called the Lagrange function and has the form of the difference between kinetic and potential energy. The necessary condition for the maximum of the functional $I[x(t)]$ has the form of equality of its first variation to zero. Based on this statement, the mathematical model of process dynamics takes the form of the Euler-Lagrange equation

$$L_x(t, x, x') - \frac{d}{dt} L_{x'}(t, x, x') = 0 \quad (3)$$

The methodology for constructing a sufficiently wide class of mathematical models is described as follows. The Lagrange function is formed on the basis of kinetic and potential energy. At the same time, the mathematical model is described by differential equations of the second order in ordinary or partial derivatives [2,9,16].

Models based on the fundamental laws of nature. The most common method of constructing models is the application of the fundamental laws of nature and a specific situation [2,16,18]. These laws are universally recognized and confirmed by history, so it is natural to use them. Such laws include, for example, the law of conservation of energy, conservation of matter, conservation of momentum, etc., and the above-mentioned laws of Newton and Hooke's law.

Application of the method of analogies. One of the approaches widely used in constructing mathematical models is the method of analogies. If, when trying to model an object, it is difficult or impossible to use the fundamental laws of nature or variational principles, then the principle of "similarity" can be used. Using analogies to previously studied phenomena is one of the fruitful approaches in modeling.

Hierarchical approach. Only in exceptional cases is it possible to construct a model in general. As a rule, due to the multifactorial nature of the process, the complexity of dependencies and the number of connections, it is impossible to do this. Therefore, the approach "from simple to complex" becomes natural. With this approach, a chain (hierarchy) of gradually increasing complexity models is built, each of which includes the previous one as a partial case.

6. Conclusions

The following results were achieved in this work:

- theoretical foundations of mathematical modeling of dynamic systems are briefly presented,
- concept of a model and mathematical model is considered,
- steps of complex process of mathematical modeling is proposed and prescribed,
- basic requirements for the mathematical model are presented,
- types of mathematical models and design methodology are considered and determined.

This article can be of interest to a wide range of scientists, beginners and experienced. It will also be very useful for university students and graduate students.

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